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Shalow acceptors in strained MQW heterostructures in strong magnetic fields

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Abstract. A new nonvariational theoretical technique allowing to calculate both ground and exited states of shallow impurity in a quantum well in the presence of strong magnetic field has been developed. The method has been applied to study the acceptor states in Ge/Ge$_{1-x}$Si$_x$ MQW heterostructures. The results obtained allow to explain the measured far IR photoconductivity spectra of the heterostructures and to identify the observed spectral lines.

Introduction

The problem of shallow impurities in multiple quantum wells (MQW) heterostructures in strong magnetic fields have been attracting the interest of researches during the last decade (see, for example, [1] and reference therein). As usual various variational methods are used for the interpretation of the experimental data. However in the most studies variational calculations are limited to consideration of the ground (1s) and the lowest exited states only because it is necessary to use trial functions with a large number of variational parameters for a satisfactory description of higher states. Sometimes it appears insufficiently for an explanation of all observed lines in the spectra of impurity absorption/photoconductivity. The technique developed in the present work is similar to that used in [2] for the calculation of the acceptor states in quantum wells structures without a magnetic field. The acceptor envelope function was expanded in the basis of Landau level wavefunctions of free holes (without the Coulomb potential) in the quantum well. By diagonalization of the acceptor Hamiltonian in this basis the series of acceptor state energies and wavefunctions was obtained, thus allowing to calculate the energies and the matrix elements of the optical transitions. The results obtained allow to interpret the observed shallow acceptor photoconductivity spectra in the far infrared range in the magnetic fields reported in [3].

1. Theoretical formalism

A calculation of the acceptor states is a rather complicated problem due to the degeneration of the valence band in semiconductors under consideration. Let's consider the problem of a hole in the impurity center Coulomb potential in a strained MQW heterostructure in strong magnetic field. The magnetic field is parallel to the growth direction. The total Hamiltonian 4×4 (without the spin-split subband terms) consists of the Luttinger Hamiltonian in the magnetic field [4], deformation terms [5], the rectangular quantum well (QW) potential and the Coulomb potential. As a first step we calculated the basis functions $\vec{\Psi}_{i,r}^{J_z}$ (the hole wave-functions in QW in the absence of the Coulomb potential). The calculations were performed using the axial approximation thus neglecting the off-diagonal elements proportional to $\gamma_2 - \gamma_3$ in the Hamiltonian, the graduation $\vec{A} = 1/2[\vec{H} \times \vec{r}]$ being chosen. The axial symmetry results in the conservation of the total angular momentum projection

on the magnetic field direction J_z. Each Landau state in the QW is characterized by the number n ($n = r + (|M| + M)/2$, $r = 0, 1, \ldots, \infty$,$M = J_z/\hbar + 3/2$), wave-function parity p and the subband number i. The Landau states prove to be degenerated on M ($M = -\infty, \ldots, -1, 0, \ldots, n$). In the above approximation the problem of the basis functions search was reduced to the solving of the system of four differential equations [6].

2. Results and discussion

In order to test the developed technique we have calculated the donor states in the GaAs/$Al_xGa_{1-x}As$ MQW. In strong magnetic fields ($H > 2$ kOe) our approach gives the results which fit the experimental data much better [7] than those obtained by the variational method [1].

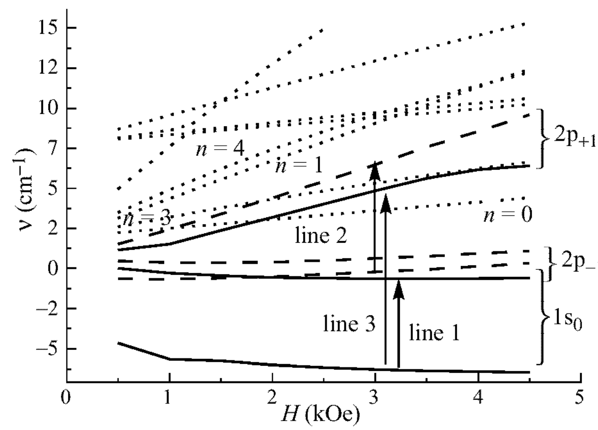

Fig. 1. Chart of calculated acceptor state energies in rectangular QW in the strained Ge/GeSi heterostructure #306 ($d_{\mathrm{GeSi}} \approx d_{\mathrm{Ge}} = 200$ Å, $\varepsilon = 2.1 \times 10^{-3}$, $x = 0.12$) vs the magnetic field. The solid lines correspond to the impurity states located in the center of QW. The dash lines refer to impurity states in the barrier center. Thin dotted lines — correspond Landau levels of free holes.

The calculation results for the ground ($1s$) and two exited ($2p_{\pm 1}$) states energies for the acceptors in the $Ge/Ge_{1-x}Si_x$ heterostructures located in the center of a QW (solid lines) and in the center of a barrier (dashed lines) are given in Fig. 1. The $2p_{\pm 1}$ states are the lowest ones to which the dipole transitions from the ground state are allowed. The Coulomb potential splits the degenerated over the M Landau states. The ground state wavefunction in strong magnetic fields is similar to that of the lowest Landau level ($n = 0$) with $J_z = -3\hbar/2$ in the first subband. It is easy to see from Fig. 1 the $2p_{-1}$ state also originate from the zeroth Landau level, however its wavefunction corresponds to the momentum projection $J_z = -5\hbar/2$. The $2p_{+1}$ state with $J_z = -1\hbar/2$ in the limit of the strong magnetic field is 'bound' to the first Landau level ($n = 1$) in the lowest subband. As one can see from Fig. 1, the impurity placed in the barrier center results in the formation of more shallow states if compared with the acceptor in the QW center. It should be mentioned, that it proved be possible to use the above method in the magnetic fields $H > 10$ kOe only. Otherwise it is necessary to increase the dimension of the basis in weaker fields significantly. The comparison of the measured and simulated FIR photoconductivity spectra in Ge/GeSi heterostructure #306 is shown in Fig. 2. The photoconductivity spectrum calculation was produced in the approach of uniform distribution of an impurity in the structure. All exited

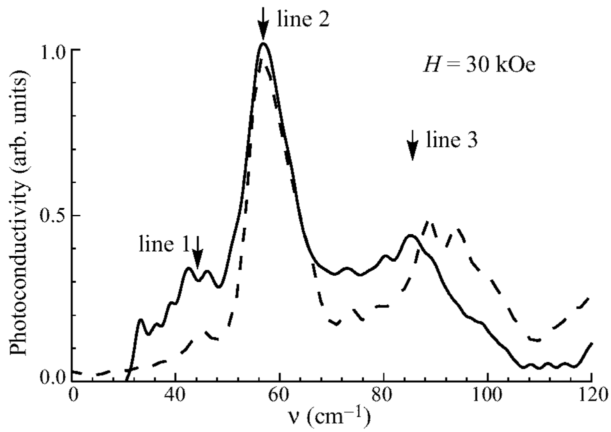

Fig. 2. Comparison of the measured and simulated FIR photoconductivity spectra in Ge/GeSi heterostructure #306. Solid line is the measured FIR photoconductivity spectra in magnetic fields. $T = 4.2$ K. Dashed curve is the simulated photoconductivity spectra for the uniform impurity distribution over the QW and the barrier.

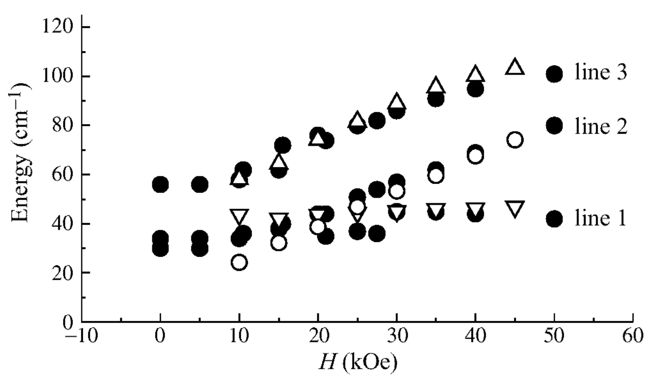

Fig. 3. Spectral positions of the measured (•) photoconductivity peaks versus the magnetic field. Signs Δ denotes $1s \to 2p_{+1}$ transition energies for well-center acceptors, O corresponds $1s \to 2p_{+1}$ transition for barrier-center acceptors, ∇ is used for $1s \to 2p_{-1}$ transition for well-center acceptors.

states, the optical transitions on which are allowed and which lay in the range up to 150 cm^{-1} were taken into account. It is necessary to note that at uniform distribution the maximal contribution to photoconductivity will be brought by transitions between states of acceptors located in the center of the quantum well and at the center of the quantum barrier. This fact is connected with the state density singularity in these places. The arrows 1, 2 and 3 in Fig. 1 indicate the optical transitions, which correspond to the observed spectral lines at the same magnetic field of 30 kOe (Fig. 2). Spectral positions of the measured photoconductivity lines on the magnetic field are shown in Fig. 3. Calculated energies of optical transitions for two acceptor positions are presented in Fig. 3 for comparison. One can easily see the good agreement between the calculated and measured data. This fact allows to unambiguously

identify these lines as the transitions $1s \rightarrow 2p_{+1}$ and $1s \rightarrow 2p_{-1}$ for the acceptor located at the center of the quantum well and $1s \rightarrow 2p_{+1}$ for the barrier-center acceptor.

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